

=> fil reg
FILE 'REGISTRY' ENTERED AT 07:34:47 ON 24 FEB 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 23 FEB 2005 HIGHEST RN 836595-43-8
DICTIONARY FILE UPDATES: 23 FEB 2005 HIGHEST RN 836595-43-8

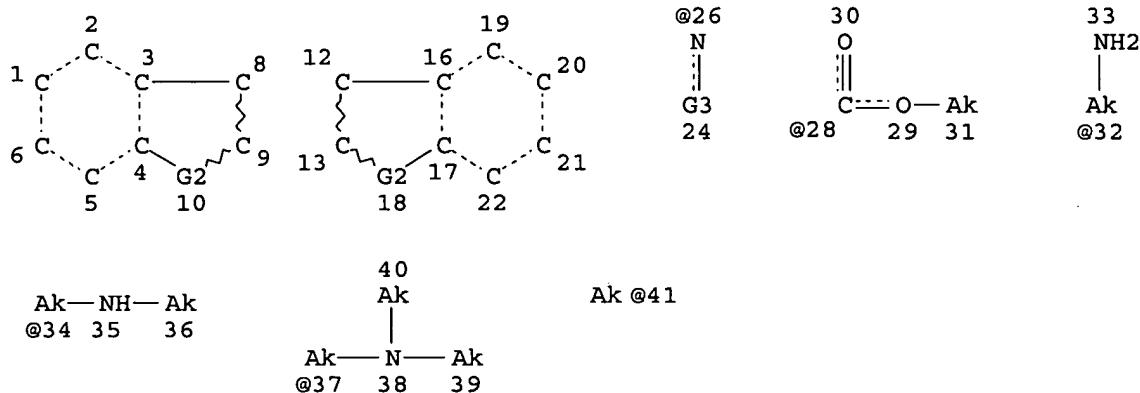
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> => d que 119
L14 STR



VAR G2=NH/26
VAR G3=41/28/32/34/37

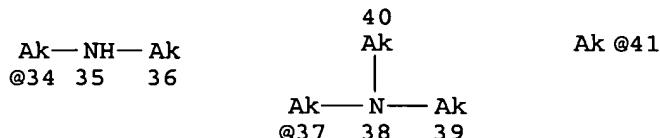
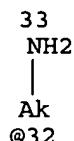
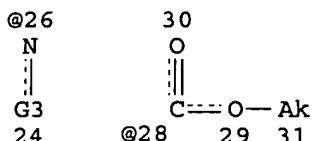
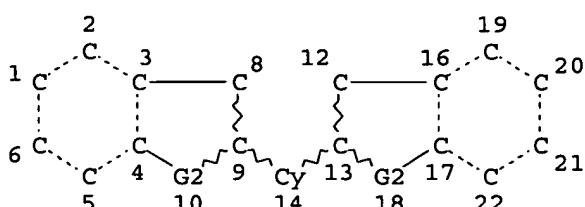
NODE ATTRIBUTES:

CONNECT IS E1 RC AT 31
CONNECT IS E2 RC AT 32
CONNECT IS E2 RC AT 34
CONNECT IS E1 RC AT 36
CONNECT IS E2 RC AT 37
CONNECT IS E1 RC AT 39
CONNECT IS E1 RC AT 40
CONNECT IS E1 RC AT 41
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE
L16 65882 SEA FILE=REGISTRY SSS FUL L14
L17 STR



VAR G2=N/26
VAR G3=41/28/32/34/37

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 31
CONNECT IS E2 RC AT 32
CONNECT IS E2 RC AT 34
CONNECT IS E1 RC AT 36
CONNECT IS E2 RC AT 37
CONNECT IS E1 RC AT 39
CONNECT IS E1 RC AT 40
CONNECT IS E1 RC AT 41
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

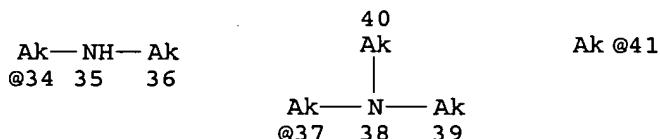
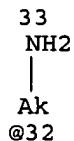
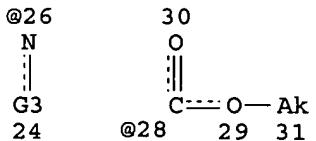
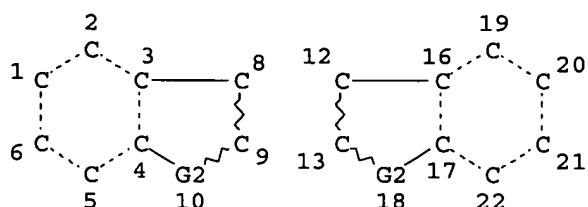
GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 35

STEREO ATTRIBUTES: NONE

L19 155 SEA FILE=REGISTRY SUB=L16 SSS FUL L17

=> d que 122
L14 STR



VAR G2=NH/26
VAR G3=41/28/32/34/37

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 31
CONNECT IS E2 RC AT 32
CONNECT IS E2 RC AT 34
CONNECT IS E1 RC AT 36

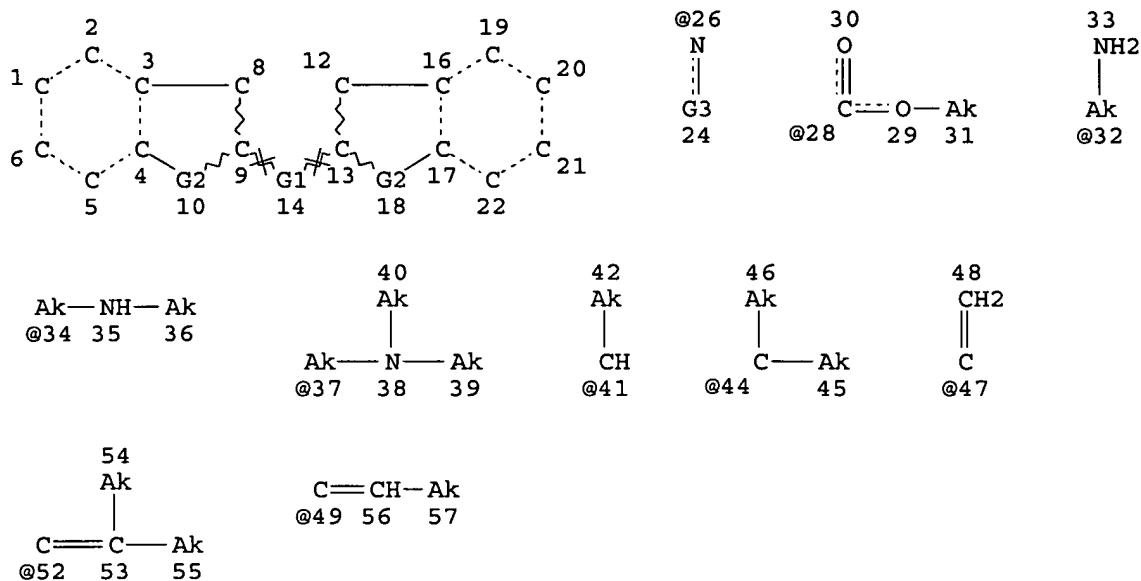
CONNECT IS E2 RC AT 37
 CONNECT IS E1 RC AT 39
 CONNECT IS E1 RC AT 40
 CONNECT IS E1 RC AT 41
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE

L16 65882 SEA FILE=REGISTRY SSS FUL L14
 L20 STR



VAR G1=O/S/CH2/41/44/47/49/52/NH/26/C/N

VAR G2=NH/26

VAR G3=AK/28/32/34/37

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

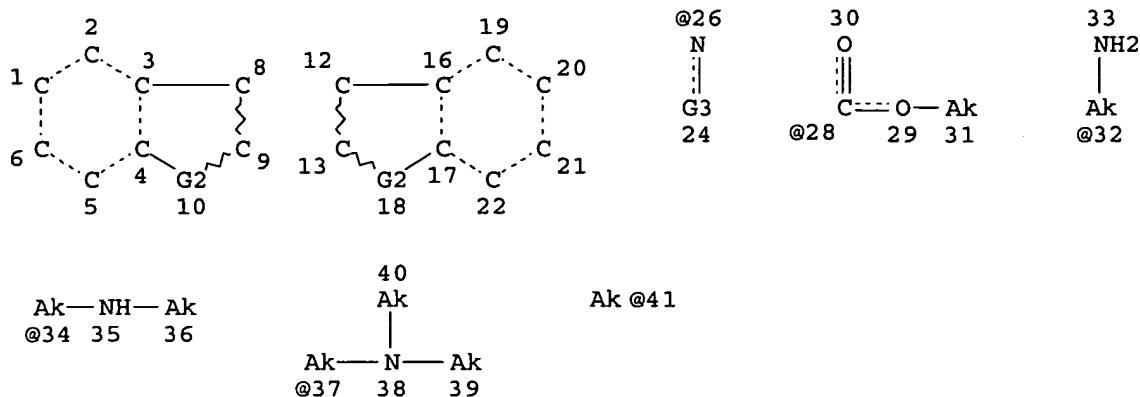
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 48

STEREO ATTRIBUTES: NONE

L22 623 SEA FILE=REGISTRY SUB=L16 SSS FUL L20

=> d que 132
 L14 STR



VAR G2=NH/26

VAR G3=41/28/32/34/37

NODE ATTRIBUTES:

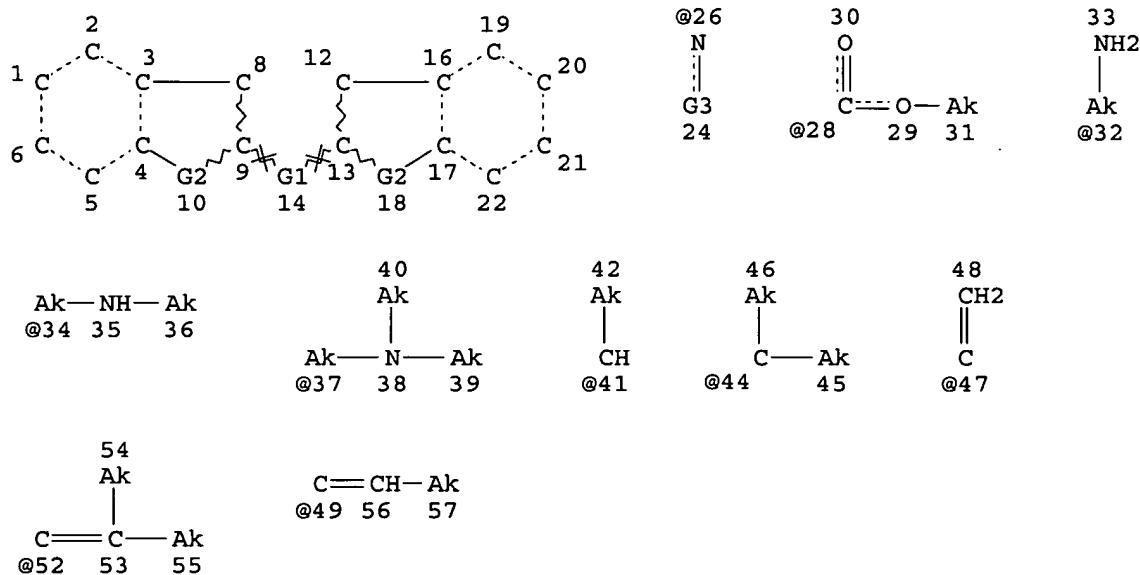
CONNECT IS E1 RC AT 31
 CONNECT IS E2 RC AT 32
 CONNECT IS E2 RC AT 34
 CONNECT IS E1 RC AT 36
 CONNECT IS E2 RC AT 37
 CONNECT IS E1 RC AT 39
 CONNECT IS E1 RC AT 40
 CONNECT IS E1 RC AT 41
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE

L16 65882 SEA FILE=REGISTRY SSS FUL L14
 L20 STR



VAR G1=O/S/CH2/41/44/47/49/52/NH/26/C/N
 VAR G2=NH/26

VAR G3=AK/28/32/34/37

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

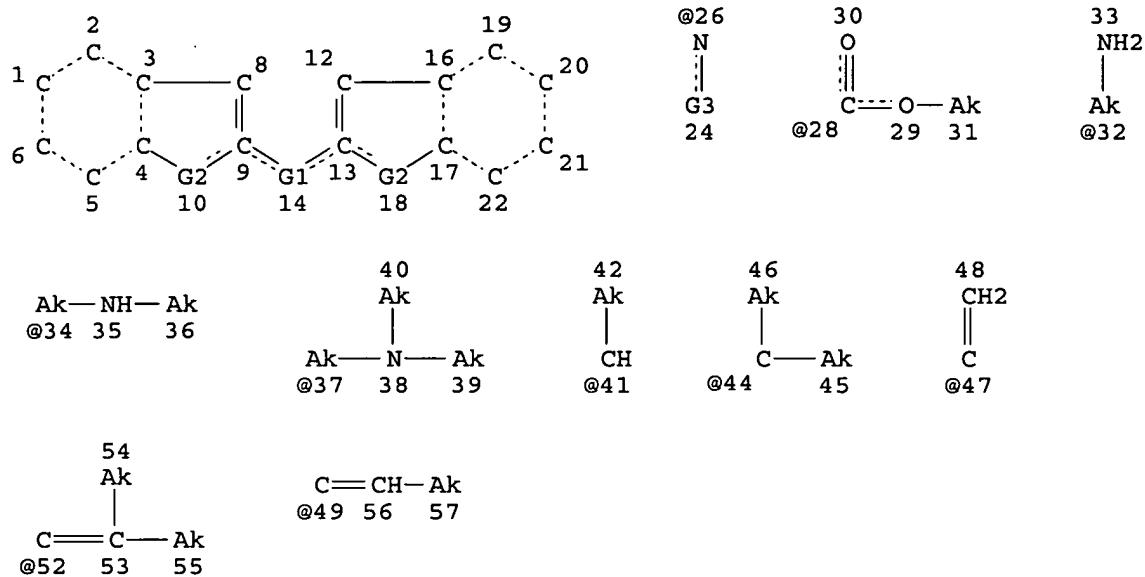
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 48

STEREO ATTRIBUTES: NONE

L22 623 SEA FILE=REGISTRY SUB=L16 SSS FUL L20
L30 STR

VAR G1=O/S/CH2/41/44/47/49/52/NH/26/C/N

VAR G2=NH/26

VAR G3=AK/28/32/34/37

NODE ATTRIBUTES:

CONNECT IS M1 RC AT 1

CONNECT IS M1 RC AT 2

CONNECT IS M1 RC AT 5

CONNECT IS M1 RC AT 6

CONNECT IS M1 RC AT 8

CONNECT IS M1 RC AT 12

CONNECT IS M1 RC AT 19

CONNECT IS M1 RC AT 20

CONNECT IS M1 RC AT 21

CONNECT IS M1 RC AT 22

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

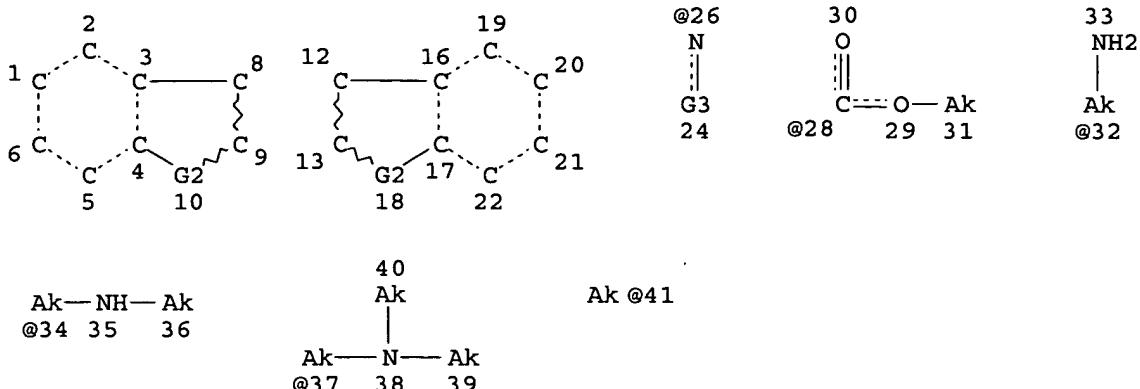
NUMBER OF NODES IS 48

STEREO ATTRIBUTES: NONE

L32 82 SEA FILE=REGISTRY SUB=L22 CSS FUL L30

=> d que 138

L14 STR



VAR G2=NH/26
VAR G3=41/28/32/34/37

NODE ATTRIBUTES:

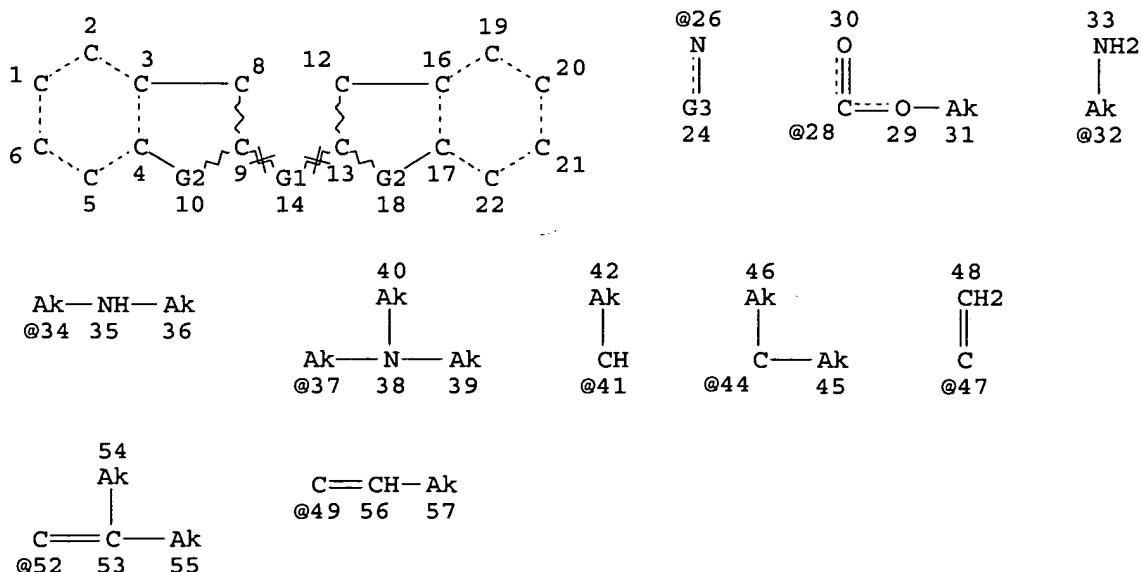
CONNECT IS E1 RC AT 31
CONNECT IS E2 RC AT 32
CONNECT IS E2 RC AT 34
CONNECT IS E1 RC AT 36
CONNECT IS E2 RC AT 37
CONNECT IS E1 RC AT 39
CONNECT IS E1 RC AT 40
CONNECT IS E1 RC AT 41
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE

L16 65882 SEA FILE=REGISTRY SSS FUL L14
L20 STR



VAR G1=O/S/CH2/41/44/47/49/52/NH/26/C/N
VAR G2=NH/26

VAR G3=AK/28/32/34/37

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

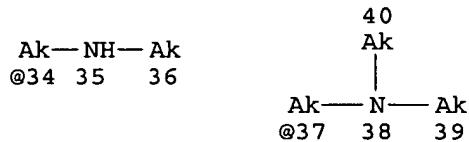
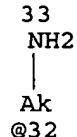
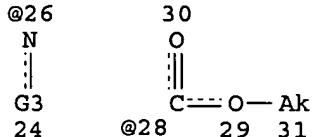
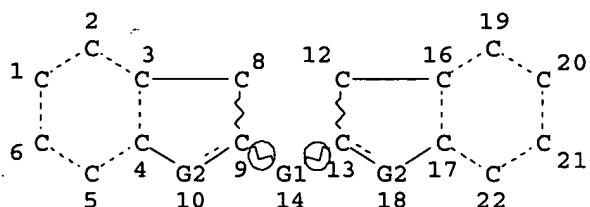
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 48

STEREO ATTRIBUTES: NONE

L22 623 SEA FILE=REGISTRY SUB=L16 SSS FUL L20
L36 STR

VAR G1=O/S/C/N

VAR G2=NH/26

VAR G3=AK/28/32/34/37

NODE ATTRIBUTES:

CONNECT IS M1 RC AT 1

CONNECT IS M1 RC AT 2

CONNECT IS M1 RC AT 5

CONNECT IS M1 RC AT 6

CONNECT IS M1 RC AT 8

CONNECT IS M1 RC AT 12

CONNECT IS M1 RC AT 19

CONNECT IS M1 RC AT 20

CONNECT IS M1 RC AT 21

CONNECT IS M1 RC AT 22

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE

L38 109 SEA FILE=REGISTRY SUB=L22 SSS FUL L36

=> d his

(FILE 'HOME' ENTERED AT 06:32:46 ON 24 FEB 2005)
SET COST OFF

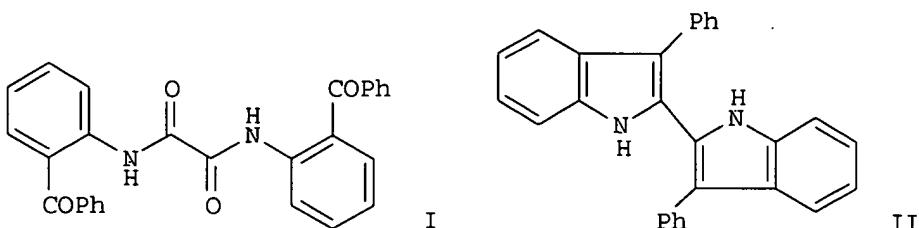
FILE 'REGISTRY' ENTERED AT 06:33:00 ON 24 FEB 2005

L1 STR

L2 1 S L1 CSS SAM

FILE 'HCAPLUS' ENTERED AT 06:41:34 ON 24 FEB 2005

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:505286 CAPLUS
DOCUMENT NUMBER: 123:83146
TITLE: Titanium-induced zipper reactions
AUTHOR(S): Fuerstner, Alois; Ptock, Arne; Weintritt, Holger;
Goddard, Richard; Krueger, Carl
CORPORATE SOURCE: Max-Planck-Inst. Kohlenforschung, Muelheim an der
Ruhr, D-45470, Germany
SOURCE: Angewandte Chemie, International Edition in English
(1995), 34(6), 678-81
CODEN: ACIEAY; ISSN: 0570-0833
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:83146
GI



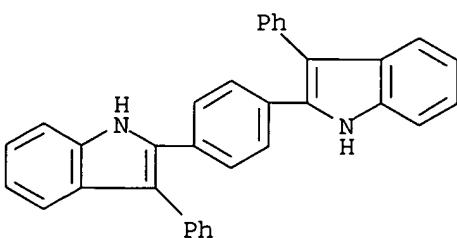
AB A one step titanium-induced zipper reaction results in an amazing and unprecedented chemo- and regioselectivity in the reductive cyclization of polycarbonyl compds. Thus, polycarbonyl compound I was treated with $TiCl_3$ and zinc dust under argon to give 80% biindole derivative II.

IT 164936-88-3P 164936-89-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(titanium-induced zipper reactions)

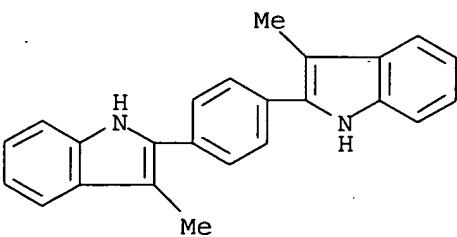
RN 164936-88-3 CAPLUS

CN 1H-Indole, 2,2'-(1,4-phenylene)bis[3-phenyl- (9CI) (CA INDEX NAME)

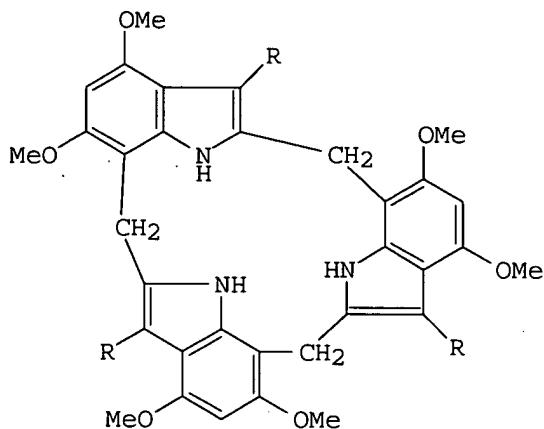


RN 164936-89-4 CAPLUS

CN 1H-Indole, 2,2'-(1,4-phenylene)bis[3-methyl- (9CI) (CA INDEX NAME)



ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1993:671129 CAPLUS
 DOCUMENT NUMBER: 119:271129
 TITLE: Calix[3]indoles, new macrocyclic
 tris(indolylmethylene) compounds with 2,7-linkages
 AUTHOR(S): Black, David S. C.; Bowyer, Michael C.; Kumar, Naresh;
 Mitchell, Peter S. R.
 CORPORATE SOURCE: Sch. Chem., Univ. New South Wales, Kensington, 2033,
 Australia
 SOURCE: Journal of the Chemical Society, Chemical
 Communications (1993), (10), 819-21
 CODEN: JCCCAT; ISSN: 0022-4936
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 119:271129
 GI



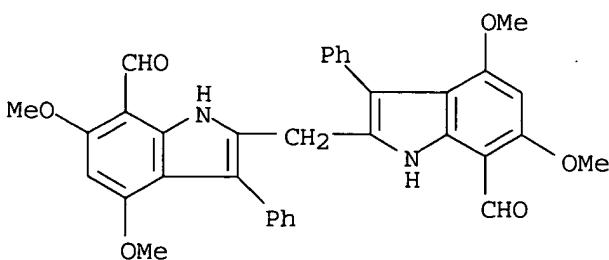
AB A series of macrocyclic tris(indolylmethylene) compds., e.g. I [R = (un)substituted Ph], can be obtained from 7- or 2-(hydroxymethyl)indoles or from the combination of either an indole with a bis(hydroxymethyl)-2,7'-diindolylmethane or a bis(hydroxymethyl)indole with a 2,7'-diindolylmethane; an isomeric series can be obtained from the combination of an indole with a bis(hydroxymethyl)-2,2'-diindolylmethane.

IT 151321-09-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reduction of)

RN 151321-09-4 CAPLUS

CN 1H-Indole-7-carboxaldehyde, 2,2'-methylenebis[4,6-dimethoxy-3-phenyl- (9CI) (CA INDEX NAME)



ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1987:617419 CAPLUS
 DOCUMENT NUMBER: 107:217419
 TITLE: Reactivity and reaction paths of methyl-substituted
 bis(indolylcarbenium) ions
 AUTHOR(S): Pindur, Ulf; Mueller, Johann
 CORPORATE SOURCE: Fachbereich Pharm., Univ. Mainz, Mainz, D-6500, Fed.
 Rep. Ger.
 SOURCE: Journal of Heterocyclic Chemistry (1987), 24(1),
 159-63
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 OTHER SOURCE(S): CASREACT 107:217419
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

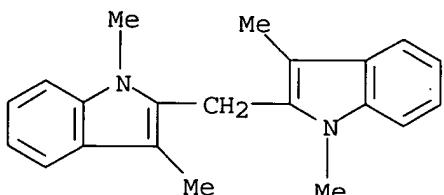
AB Me substituted bisindolylcarbenium ions I and II (R = H, Me) react with some O- and C-nucleophiles regioselectively. The cations II yield with hydroxide ions the tetraindolylidimethyl ether III and with methoxide ions the bisindolylmethoxymethanes IV. I and II react with several methylindoles to give isomeric bis- and trisindolylmethanes. An electrophilic reactivity order of cations I and II can be derived from the exptl. results.

IT 91455-03-7P 110968-29-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

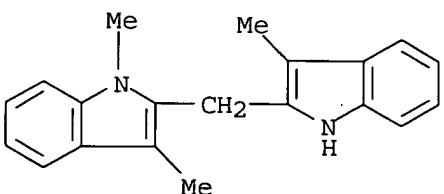
RN 91455-03-7 CAPLUS

CN 1H-Indole, 2,2'-methylenebis[1,3-dimethyl- (9CI) (CA INDEX NAME)

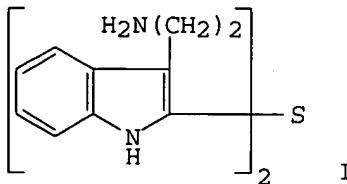


RN 110968-29-1 CAPLUS

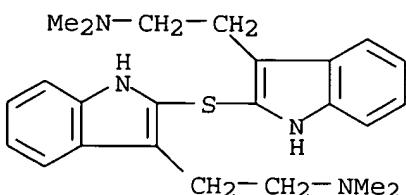
CN 1H-Indole, 1,3-dimethyl-2-[(3-methyl-1H-indol-2-yl)methyl]- (9CI) (CA INDEX NAME)



ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1985:184940 CAPLUS
 DOCUMENT NUMBER: 102:184940
 TITLE: A novel serotonin antagonist 2,2'-bis[3-(2-N,N-dimethylaminoethyl)indolyl]sulfide (BDIS)
 AUTHOR(S): Chu, C. K.; Wander, J. D.; Tackett, R. L.; Iturrian, W. B.; Schmitz, J. P.; Garner, G. E.; Chae, K.
 CORPORATE SOURCE: Coll. Pharm., Univ. Georgia, Athens, GA, 30602, USA
 SOURCE: Journal of Heterocyclic Chemistry (1984), 21(6), 1901-3
 DOCUMENT TYPE: CODEN: JHTCAD; ISSN: 0022-152X
 LANGUAGE: English
 GI

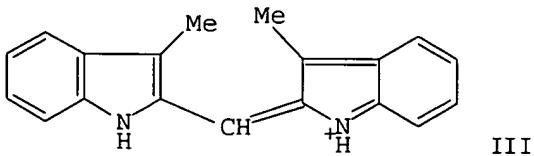
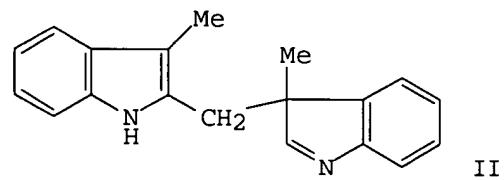
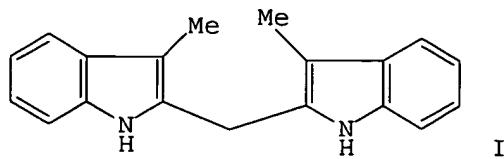


AB A novel serotonin antagonist, 2,2'-bis[3-(2-N,N-dimethylaminoethyl)indolyl]sulfide (I) was synthesized in 1 step from the reaction of N,N-dimethyltryptamine with SO₂Cl₂.
 IT 96249-78-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 96249-78-4 CAPLUS
 CN 1H-Indole-3-ethanamine, 2,2'-thiobis[N,N-dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)

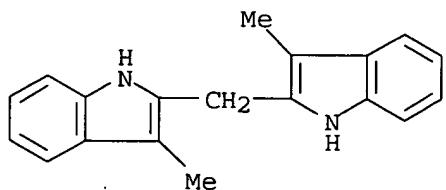


● HCl

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1980:471451 CAPLUS
 DOCUMENT NUMBER: 93:71451
 TITLE: 2,3'-Bis(3-methylindolyl)methane from 3-methylindole
 and formaldehyde
 AUTHOR(S): Brieskorn, Carl Heinz; Huber, Johannes
 CORPORATE SOURCE: Inst. Pharm. Lebensmittelchem., Univ. Wuerzburg,
 Wuerzburg, D 8700, Fed. Rep. Ger.
 SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1979),
 312(12), 1046-51
 DOCUMENT TYPE: CODEN: ARPMAS; ISSN: 0365-6233
 LANGUAGE: Journal
 German
 GI



AB Hopkins-Cole reaction of 3-methylindole with H₂CO in MeOH-H₂SO₄ gave I and II. II is the precursor of ion III, the color product of this reaction.
 IT 36798-17-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 36798-17-1 CAPLUS
 CN 1H-Indole, 2,2'-methylenebis[3-methyl- (9CI) (CA INDEX NAME)



ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1975:111897 CAPLUS
DOCUMENT NUMBER: 82:111897
TITLE: Reaction of skatole with iodine in the presence of thiourea
AUTHOR(S): Hino, Tohru; Endo, Mamoru; Nakagawa, Masako
CORPORATE SOURCE: Fac. Pharm. Sci., Chiba Univ., Chiba, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1974), 22(11), 2728-31
CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

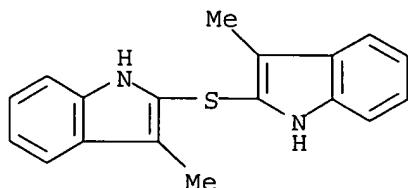
AB Skatole was treated with iodine and H₂NCSNH₂ in EtOH containing KI to give the indoles I (11.6%), II (23%), and III (13%), 3.4% 3-methyloxindole, 3-methyldioxindole (trace), and 2.2% bis(3-methyl-2-indolyl) sulfide. I also was prepared by treating 2-bromoskatole with H₂N-CSNH₂-HBr followed by KI.

IT 55132-21-3P

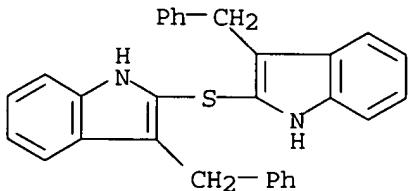
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 55132-21-3 CAPLUS

CN 1H-Indole, 2,2'-thiobis[3-methyl- (9CI) (CA INDEX NAME)



ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1974:59818 CAPLUS
DOCUMENT NUMBER: 80:59818
TITLE: Preparation of 3-substituted 2-indolinethiones via
diindolyl disulfides. Reaction of 3-substituted
indoles with sulfur monochloride
AUTHOR(S): Hino, Tohru; Suzuki, Toshikazu; Takeda, Sachie; Kano,
Nobuko; Ishii, Yoichi; Sasaki, Akira; Nakagawa, Masako
CORPORATE SOURCE: Fac. Pharm. Sci., Chiba Univ., Chiba, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1973), 21(12),
2739-48
DOCUMENT TYPE: CODEN: CPBTAL; ISSN: 0009-2363
LANGUAGE: Journal
English
GI For diagram(s), see printed CA Issue.
AB The reaction of 3-alkylindoless (I) with S₂Cl₂ in ether gave the
corresponding 2-diindolyl disulfides (II, n = 2) as the main product, and
mono- and trisulfides (I, n = 1,3) as minor products. The similar
reaction of 3-arylindoless gave the disulfides in good yields. Reduction of
the diindolyl disulfides with NaBH₄ in EtOH afforded the 2-indolinethiones
(III) in good yields.
IT 51206-69-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reduction of, indolinethiones by)
RN 51206-69-0 CAPLUS
CN 1H-Indole, 2,2'-thiobis[3-(phenylmethyl)- (9CI) (CA INDEX NAME)



ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1972:405277 CAPLUS
 DOCUMENT NUMBER: 77:5277
 TITLE: Light-induced reactions of α -(N-alkylanilino) ketones. Formation of diindolylmethanes
 AUTHOR(S): Hill, J.; Townend, J.
 CORPORATE SOURCE: Dep. Chem., Univ. Salford, Salford, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1972), (9-10), 1210-19
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Irradiation of 6 α -(N-alkylanilino) ketones, $\text{PhN}(\text{CH}_2\text{R})\text{CHR}_1\text{COMe}$ (I; R, R_1 = H, Me, or Ph), in MeOH, Me_2CHOH , or benzene caused fission of the α -C-N bond giving a secondary amine (PhNHCH_2R), a ketone ($\text{R}_1\text{CH}_2\text{COMe}$), an α -[p-(alkylamino)phenyl] ketone formed by para rearrangement, and a substituted 2-methylindole formed by ortho rearrangement with subsequent cyclodehydration. I ($\text{R}_1 = \text{H}$) also gave a diindol-3-ylmethane derived from the 2-methylindole. Irradiation of I with 1,2-dimethylindole gave diindolylmethanes, via 1-phenylazetidinols as labile intermediates. Irradiation of 7 anilino ketones $\text{PhNRCH}_2\text{COR}_1$ ($\text{R} = \text{H}$, Me, or Me_3C ; $\text{R}_1 = \text{Me}$, Et, Me_3C , or Ph) was also studied.
 IT 36798-56-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 36798-56-8 CAPLUS
 CN 1H-Indole, 2,2'-methylenebis[3-ethyl-1-methyl- (9CI) (CA INDEX NAME)

